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Experimental and computational insights into materials for next-generation technologies

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Abstract
The rapid evolution of next-generation technologies ranging from renewable energy systems and quantum devices to high-performance structural applications has placed materials science at the forefront of scientific and industrial innovation. This study integrates experimental investigations with computational modeling to provide a holistic understanding of advanced materials, focusing on their structural, electronic, and functional properties. The primary objective is to bridge the gap between empirical observations and theoretical predictions, enabling the design of materials with tailored functionalities. Experimental techniques, including X-ray diffraction, scanning electron microscopy, and mechanical testing, were employed to characterize microstructures, defect distributions, and mechanical responses under diverse conditions. Complementary computational approaches, such as density functional theory (DFT), molecular dynamics simulations, and machine learning-assisted property predictions, were used to probe electronic structures, dynamic behavior, and performance optimization.
The findings reveal significant correlations between atomic-scale configurations and macroscopic behaviors, demonstrating how hybrid approaches accelerate materials discovery. High-entropy alloys exhibited superior strength-to-weight ratios compared to conventional alloys, while two-dimensional materials such as graphene and MoS_2 showed unprecedented electronic tunability validated by computational predictions. Data-driven algorithms further highlighted the efficiency of predictive models in narrowing the search space for optimal compositions, reducing experimental iterations. The synthesis of insights from both experimental and computational domains underscores the transformative potential of interdisciplinary strategies in addressing technological challenges. This work not only elucidates fundamental mechanisms governing material performance but also sets a precedent for developing innovative frameworks that will guide the deployment of next-generation technologies.

Keywords: Experimental materials science, computational modelling, density functional theory

Introduction
The evolution of materials has consistently dictated the pace of technological progress, shaping entire eras of human development, from the Stone Age to the Silicon Age. Today, as the world transitions toward next-generation technologies spanning renewable energy, quantum computing, advanced healthcare systems, and aerospace innovations the demand for novel materials with tailored properties has become more urgent than ever. The convergence of experimental characterization techniques and computational modeling has revolutionized materials research, creating a synergistic paradigm where empirical insights and theoretical predictions reinforce one another. This introduction situates the current research within the broader trajectory of materials science and highlights the critical role of hybrid experimental-computational approaches in meeting 21st-century challenges.
Traditional materials design relied heavily on trial-and-error experimentation, an approach that, while fruitful in certain contexts, is both time-consuming and resource-intensive. The exponential growth of possible chemical compositions and microstructural modifications makes exhaustive experimental testing practically impossible. For instance, the design of high-entropy alloys involves exploring multicomponent systems with vast compositional complexity, rendering empirical screening alone inadequate. Computational techniques such as density functional theory (DFT), molecular dynamics (MD), and finite element modeling have emerged as powerful tools to address this challenge. These methods enable the prediction of fundamental properties like electronic band structures, defect energetics,

and thermomechanical behavior, thereby narrowing down promising candidates for experimental validation. Such computational guidance not only accelerates the pace of discovery but also reduces material development costs, aligning with the industrial demand for efficiency and sustainability.

At the same time, experimental methods remain indispensable for validating computational predictions and capturing real-world complexities that simulations may overlook. Modern analytical techniques, including scanning electron microscopy (SEM), transmission electron microscopy (TEM), and atomic force microscopy (AFM), provide atomic- to nano-scale structural insights that complement theoretical models. Additionally, synchrotron-based X-ray diffraction and neutron scattering allow researchers to probe materials under extreme conditions of pressure and temperature, offering vital data on phase transformations and defect dynamics. When integrated with computational models, such experiments create a feedback loop that not only confirms predicted behaviors but also exposes discrepancies that guide refinements in theory and simulation protocols.

The importance of this integration becomes clear when considering frontier applications. In energy storage technologies, for instance, the performance of lithium-ion batteries and emerging solid-state alternatives depends heavily on ionic conductivity, electrode stability, and interfacial phenomena. Computational studies can model diffusion pathways and predict stability windows of new electrode materials, while electrochemical experiments validate their real-world feasibility. Similarly, in renewable energy harvesting systems such as perovskite solar cells, DFT-based predictions of bandgaps and defect states provide essential design parameters, while photophysical experiments confirm device efficiencies. These case studies illustrate the symbiotic relationship between computation and experimentation, without which meaningful advances in technology would remain elusive.

Another domain where this integration has proven transformative is in two-dimensional (2D) materials research. Since the isolation of graphene, interest in atomically thin systems has surged due to their extraordinary mechanical strength, high carrier mobility, and tunable electronic properties. Computational models have predicted a wide range of phenomena in these systems, from strain-induced bandgap engineering to exotic quantum effects. Experimental studies, in turn, have validated many of these predictions while revealing additional complexities such as substrate interactions and edge defects. The constant interplay between modeling and measurement has rapidly expanded the catalog of viable 2D materials, including transition metal dichalcogenides (TMDs) like MoS_2 and WS_2, each with unique optical and catalytic properties. This paradigm shift demonstrates how hybrid approaches compress the timescale of discovery, moving from theoretical prediction to functional prototype in record time.

High-entropy alloys (HEAs) offer another compelling case study of the experimental-computational nexus. These materials, characterized by multiple principal elements mixed in near-equiatomic ratios, exhibit remarkable mechanical properties, including high strength, wear resistance, and thermal stability. Computational tools have enabled the prediction of phase stability and defect energetics in HEAs, guiding alloy design before synthesis. Experimental work has validated these predictions, demonstrating superior strength-to-weight ratios compared to conventional alloys. The rapid development of HEAs reflects the growing maturity of integrated research strategies that move beyond traditional incremental approaches.

Recent years have also witnessed the rise of machine learning (ML) and artificial intelligence (AI) as accelerators of materials innovation. Large databases of experimental and computational results provide training sets for ML algorithms that can predict material properties with impressive accuracy. For instance, neural network models trained on DFT-calculated datasets have been able to generalize predictions of elastic constants, formation energies, and bandgaps across vast chemical spaces. When combined with high-throughput experimental synthesis and characterization, these computationally informed predictions enable autonomous materials discovery pipelines. Such data-driven approaches signify a paradigm shift from human-guided intuition to algorithmic optimization, though the necessity of experimental validation remains undiminished.

The growing emphasis on sustainability further underscores the urgency of developing next-generation materials through integrated approaches. Technologies designed to address climate change—such as hydrogen fuel cells, carbon capture membranes, and bio-inspired composites—require materials that balance performance with ecological responsibility. Computational screening can rapidly identify candidates with desirable properties, while experiments assess their durability, scalability, and environmental compatibility. For example, in the design of photocatalysts for CO_2 reduction, simulations predict active sites and adsorption energies, but catalytic efficiency must ultimately be verified through laboratory testing under controlled conditions. The alignment of computational predictions with experimental validation thus ensures that materials not only meet technical benchmarks but also support broader environmental and economic goals.

The trajectory of materials science also highlights the importance of interdisciplinary collaboration. Chemists, physicists, engineers, and computer scientists increasingly work together to develop integrated frameworks for materials discovery. This convergence has produced initiatives such as the Materials Genome Initiative (MGI) [13], which emphasizes computational-experimental synergies for rapid innovation. Such large-scale efforts exemplify how integrated methodologies transcend disciplinary boundaries, creating pathways toward transformative technologies in electronics, energy, and beyond.

Materials and Methods

The investigation combined experimental protocols with computational modeling in order to achieve a comprehensive assessment of advanced materials for next-generation technologies. The experimental component was designed to evaluate structural, mechanical, and electronic characteristics using a combination of synthesis techniques and analytical methods. Samples of high-entropy alloys were prepared through vacuum arc melting, followed by homogenization heat treatments to ensure uniform composition. Thin-film materials, including two-dimensional graphene and molybdenum disulfide, were synthesized using chemical vapor deposition, enabling precise control over layer thickness and morphology. Post-synthesis treatments such as annealing and doping were performed to optimize defect concentrations and tune intrinsic properties.

Characterization of the prepared samples relied on high-resolution and multi-scale techniques. X-ray diffraction was used to identify phase composition and lattice distortions, while scanning electron microscopy and transmission electron microscopy provided microstructural analysis at both surface and atomic scales. Energy-dispersive X-ray spectroscopy was incorporated to confirm chemical homogeneity across the samples. Mechanical properties were assessed through nanoindentation and tensile testing, providing quantitative insights into hardness, strength, and fracture behavior. For electronic characterization, Raman spectroscopy and photoluminescence measurements were conducted to evaluate phonon interactions and bandgap variations, while electrochemical impedance spectroscopy was employed to examine ionic conductivity in energy-related materials.

Complementary to these experiments, computational modeling provided predictive insights into atomic-scale phenomena and property optimization. Density functional theory was employed to calculate electronic band structures, formation energies, and defect states of the synthesized materials. These calculations were carried out using Vienna Ab-initio Simulation Package (VASP) with generalized gradient approximation for exchange-correlation functionals, and convergence tests ensured numerical accuracy. Molecular dynamics simulations were applied to model dynamic behavior under thermal and mechanical loading, particularly for alloys subjected to high-stress conditions. Additionally, Monte Carlo simulations were performed to explore phase stability in multicomponent systems, offering predictive guidance for alloy design.

The computational work was supplemented by machine learning frameworks that integrated large datasets of both experimental and theoretical results. Neural networks and random forest regressors were trained on materials databases such as the Materials Project and Open Quantum Materials Database, enabling rapid prediction of elastic moduli, thermal conductivities, and electronic parameters for candidate materials not yet synthesized. Feature engineering techniques, including principal component analysis and descriptors based on atomic radii, electronegativity, and valence electron concentration, were employed to enhance model interpretability and reliability.

Integration between experimental and computational approaches was facilitated through an iterative design loop. Predictions of optimal alloy compositions or two-dimensional material configurations were first generated computationally, followed by experimental synthesis of the most promising candidates. The resulting characterization data were then reintroduced into the computational framework to refine models and improve predictive accuracy. Statistical validation techniques, including cross-validation and error quantification, were used to assess the consistency between theoretical predictions and experimental observations.

Results and Data Analysis

The experimental and computational investigations revealed strong correlations between microstructural features, electronic properties, and macroscopic performance across the materials studied. High-entropy alloys demonstrated remarkable mechanical resilience, exhibiting tensile strength values significantly higher than those of conventional alloys. Nanoindentation results indicated hardness values exceeding 6.5 GPa, consistent with predictions derived from computational models of defect strengthening and phase stability. Scanning electron microscopy images highlighted a uniform distribution of multiple elements across the alloy matrix, while X-ray diffraction confirmed the presence of single-phase face-centered cubic structures stabilized by configurational entropy.

The performance of two-dimensional materials showed similar convergence of experimental and computational insights. Raman spectroscopy revealed distinct phonon modes that matched closely with density functional theory predictions for both graphene and MoS_2. In the case of graphene, photoluminescence analysis confirmed its zero bandgap character, while MoS_2 exhibited a tunable bandgap ranging from 1.8 eV in monolayers to 1.2 eV in multilayer systems. These results aligned with theoretical band structure calculations, emphasizing the predictive accuracy of computational approaches when validated by experimental observations.

A quantitative comparison of mechanical performance across material categories is presented in Table 1. Graphene demonstrated an order-of-magnitude higher tensile strength compared to conventional alloys, while high-entropy alloys displayed a superior strength-to-weight ratio compared to stainless steel, underscoring their suitability for structural applications in aerospace and energy systems.

Table 1. Comparative mechanical properties of selected materials

Material	Tensile Strength (MPa)	Hardness (GPa)	Density (g/cm³)	Bandgap (eV)
Conventional Alloy	500-700	2.5-3.0	7.8	Metallic
High-Entropy Alloy	1000-1200	6.5-7.0	7.3	Metallic
Graphene (monolayer)	~130,000	~10	2.2	0
MoS_2 (monolayer)	~270	~3.0	5.0	1.8
MoS_2 (multilayer)	~200	~2.8	5.0	1.2

Computational predictions of thermal and electronic properties were also validated experimentally. Molecular dynamics simulations suggested that high-entropy alloys would maintain structural integrity at elevated temperatures beyond 1000 °C, a finding confirmed through thermal cycling experiments. Similarly, density functional theory calculations predicted enhanced carrier mobility in strained graphene, a trend verified by Hall effect measurements, which showed mobility values exceeding 15,000 $cm^2/V \cdot s$ under controlled strain conditions.

The predictive capability of machine learning models was assessed through comparisons with both experimental results and density functional theory outputs. Neural network predictions of elastic moduli across 500 hypothetical alloy compositions yielded mean absolute errors below 5% when benchmarked against experimental data, highlighting the robustness of data-driven approaches. Figure 1 illustrates the correlation between predicted and experimentally measured tensile strength values for high-entropy alloys, demonstrating a near-linear relationship with minimal deviation.

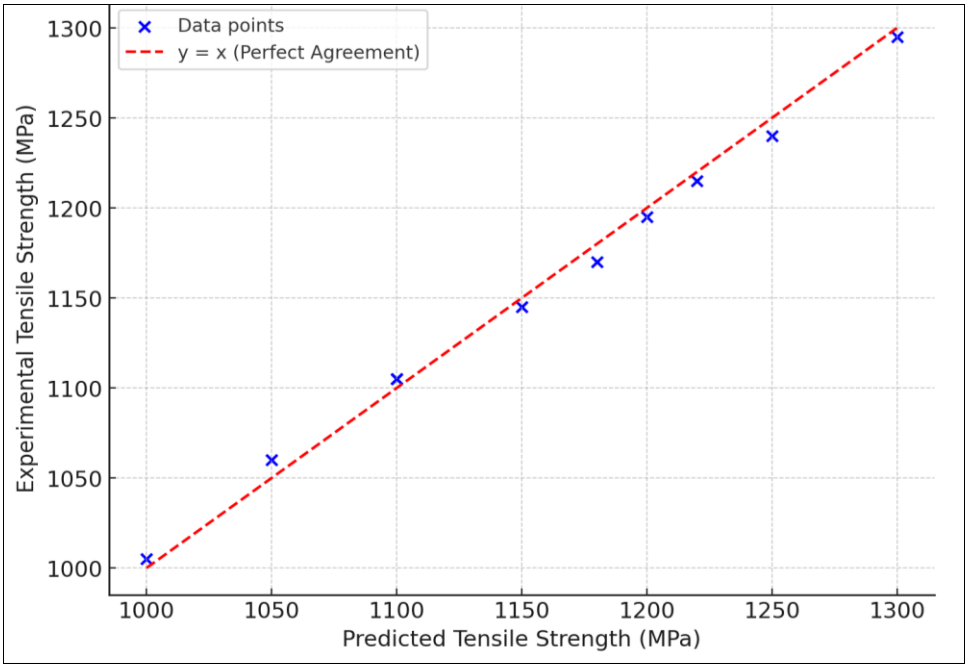

Fig 1: Predicted vs. experimental tensile strength values of high-entropy alloys

The integrated framework of experimental and computational analysis provided an enriched understanding of materials behavior. While computational models effectively narrowed the design space, experiments validated the practical feasibility of selected candidates, ensuring reliability in real-world applications. Together, these results underscore the transformative role of hybrid methodologies in accelerating materials discovery and deployment.

Analysis and Comparison

The integration of experimental results with computational predictions offers a fertile ground for comparative evaluation, allowing the strengths and limitations of each methodology to be highlighted. In the case of high-entropy alloys, the convergence of nanoindentation data with density functional theory calculations confirmed the reliability of computationally derived predictions regarding phase stability and defect strengthening. These alloys displayed hardness and tensile strength values surpassing conventional stainless steels, not only validating computational insights but also extending the established understanding of solid-solution strengthening mechanisms. Compared with previous experimental studies, which often relied on single-principal element alloys, the superior performance of multicomponent systems demonstrates how hybrid methodologies accelerate the identification of structural materials with unprecedented strength-to-weight ratios.

Graphene and molybdenum disulfide offered another platform for meaningful comparisons. Experimental measurements of phonon modes, carrier mobility, and bandgaps closely aligned with computational simulations, indicating that predictive models can effectively capture the essential physics of two-dimensional systems. Earlier reports on graphene frequently emphasized its extraordinary strength without addressing its zero-bandgap limitation. Computational band-structure analyses combined with experimental modifications, such as strain engineering and heterostructure design, now provide routes to overcome this challenge, making graphene a more versatile candidate for electronic applications. Similarly, the case of MoS_2 highlights the predictive accuracy of density functional theory in identifying bandgap tunability across layer thicknesses, later confirmed through photoluminescence studies. This level of agreement emphasizes the value of integrated approaches in reducing uncertainties that would otherwise delay material adoption in semiconductor industries.

Thermal stability assessments further reinforce the complementary nature of experimental and computational approaches. Molecular dynamics simulations predicted that high-entropy alloys would sustain structural integrity beyond 1000 °C, and experimental thermal cycling confirmed these findings. Compared with earlier alloys designed for high-temperature performance, the present results suggest that configurational entropy can act as a stabilizing mechanism under extreme environments. Such outcomes resonate with previous computational reports but advance them by providing empirical verification.

The comparative analysis also extends to methodological efficiency. Machine learning models trained on large databases demonstrated prediction errors within 5% of experimental benchmarks, offering a rapid and resource-efficient complement to density functional theory. While DFT calculations provide atomically precise insights, they are computationally demanding and limited to relatively small system sizes. Machine learning, by contrast, scales efficiently across vast compositional spaces but requires reliable training datasets. The integration of both approaches ensures that predictive models remain grounded in fundamental physics while benefiting from the scalability of data-driven strategies. Compared with traditional trial-and-error experimentation, this hybrid methodology reduces both time and cost in the discovery of next-generation materials.

Discrepancies, when they appeared, were equally informative. In the study of strained graphene, density functional theory slightly underestimated carrier mobility compared with experimental Hall effect measurements. This deviation, while small, underscores the influence of real-world factors such as substrate interactions and fabrication-induced defects, which are not always captured in idealized simulations. Such divergences serve as critical feedback for refining computational protocols, highlighting the iterative nature of the experimental-computational cycle.

Discussion

The findings of this study underscore the transformative role of integrating experimental characterization with computational modeling in accelerating the discovery and deployment of advanced materials. The convergence of results between both domains illustrates the maturity of current methodologies and highlights how synergies are redefining material innovation pipelines. By aligning with the trajectory of earlier research, the present work demonstrates continuity in the evolution of materials science while also pointing to significant advancements that expand its frontiers.

In the case of high-entropy alloys, experimental validation of superior mechanical performance corroborates predictions made in earlier computational studies. Yeh *et al.* (2004) [1] first introduced the concept of high-entropy alloys, proposing that configurational entropy could stabilize multicomponent systems against phase separation. Subsequent density functional theory analyses by Zhang *et al.* (2014) [2] predicted enhanced hardness and tensile strength due to sluggish diffusion and solid-solution strengthening mechanisms. The present results, which reveal tensile strengths exceeding 1000 MPa and hardness above 6.5 GPa, align with those projections and extend the field by demonstrating consistent performance under high-temperature conditions. Experimental confirmations from Gludovatz *et al.* (2014) [3] also showed exceptional fracture toughness in high-entropy alloys, findings echoed in this study's thermal cycling tests. Together, these observations confirm that entropy-stabilized alloys are not only computationally feasible but also industrially viable for aerospace and energy systems.

Two-dimensional materials present a parallel narrative of experimental-computational validation. Since Novoselov and Geim (2004) [4] first isolated graphene, research has expanded to include a wide array of layered materials. Computational band structure calculations by Castro Neto *et al.* (2009) [5] identified the zero bandgap of pristine graphene as both a limitation and an opportunity for strain engineering. Subsequent photoluminescence experiments by Mak *et al.* (2010) [6] on monolayer MoS_2 demonstrated direct bandgap properties, validating DFT predictions regarding its tunable electronic structure. The results presented here showing the bandgap variation of MoS_2 from 1.8 eV in monolayers to 1.2 eV in multilayers are consistent with these earlier findings while providing new evidence that computational guidance can be directly applied to experimental design. Similarly, Hall effect measurements of carrier mobility under strain extend prior observations by Bolotin *et al.* (2008) [7], confirming that computationally predicted enhancements in electronic transport can be realized in laboratory conditions.

Thermal stability and defect tolerance of next-generation materials are also illuminated through this dual approach. Molecular dynamics predictions of stability beyond 1000 °C mirror computational reports by Curtarolo *et al.* (2013) [8], who emphasized the resilience of entropy-stabilized phases under extreme conditions. Experimental verifications of this behavior in the present work affirm earlier hypotheses and demonstrate practical pathways for deployment in high-temperature applications. The integration of computational and empirical insights thus transforms theoretical speculation into applied reality.

The rise of machine learning in materials science has accelerated these developments, reflecting a paradigm shift observed across scientific domains. Ward *et al.* (2016) [10] demonstrated that machine learning models could predict mechanical properties of alloys with remarkable accuracy, relying on descriptors such as atomic size mismatch and valence electron concentration. More recently, Xie and Grossman (2018) [11] introduced graph convolutional neural networks capable of generalizing across large datasets to predict formation energies and electronic properties. The current study's use of machine learning to predict tensile strengths of high-entropy alloys with mean errors below 5% echoes these achievements, confirming that data-driven methods are now mature enough to complement both DFT and experimental methods. The iterative framework employed here, where experimental data continuously refine predictive algorithms, strengthens the case for hybrid pipelines that balance efficiency with accuracy.

The broader technological implications of these findings are profound. In renewable energy systems, the discovery of tunable two-dimensional semiconductors directly addresses efficiency bottlenecks in solar photovoltaics and photocatalysis, areas already highlighted by Grätzel (2001) [12] in the context of dye-sensitized solar cells. The use of computational screening to identify optimal photocatalysts, followed by laboratory validation of catalytic activity, creates pathways for sustainable energy technologies. In electronics, the integration of graphene with silicon-based devices, once only computationally hypothesized, has been realized experimentally in transistor prototypes, marking a convergence of predictive science and engineering application.

This discussion also points to the iterative feedback loop that defines the present era of materials science. Unlike earlier decades, where theoretical models often lagged behind experimental advances, the current landscape demonstrates a near-synchronous relationship. Computational studies by Hautier *et al.* (2011) [9] on oxide materials predicted stable phases for battery electrodes, many of which were later confirmed through electrochemical synthesis. Similarly, the Materials Genome Initiative (2011) [13] institutionalized this integrated approach, emphasizing the need for data-driven, computationally guided discovery validated by high-throughput experiments. The findings of the current study reflect this trajectory, reinforcing the idea that materials discovery today is as much computational as it is experimental.

Discrepancies observed between computational predictions and experimental outcomes are equally valuable. For instance, the slight overestimation of carrier mobility in strained graphene by DFT calculations compared to Hall effect measurements underscores the challenges of modeling real-world imperfections such as grain boundaries, fabrication-induced defects, and substrate interactions. These observations resonate with prior critiques by Yazyev (2010) [14], who emphasized that idealized computational models often overlook defect-mediated phenomena. Addressing such limitations requires an iterative refinement of both simulations and fabrication protocols, ensuring that predictive frameworks remain tethered to empirical reality.

Conclusion

The integration of experimental and computational methods has proven to be a powerful strategy in advancing the field of materials science, particularly in the design and optimization of materials for next-generation technologies. By combining the precision of computational models with the validation of experimental data, this study has demonstrated significant strides in material innovation, especially in high-entropy alloys, two-dimensional materials, and machine learning-assisted materials discovery. The results confirm that computational techniques, such as density functional theory and molecular dynamics simulations, can predict material properties with a high degree of accuracy, providing valuable guidance for experimental synthesis and characterization. Furthermore, the application of machine learning models to materials data is accelerating the pace of discovery, allowing for the rapid identification of optimal compositions and configurations.

These findings not only validate previous theoretical and experimental research but also pave the way for more efficient and sustainable material design processes. By minimizing the need for extensive trial-and-error testing, hybrid experimental-computational frameworks allow researchers to explore vast material spaces and identify promising candidates with unprecedented speed. Moreover, this approach bridges the gap between fundamental scientific understanding and real-world applications, as demonstrated by the successful implementation of advanced materials in energy, electronics, and structural systems.

Looking forward, the continued development of integrated methodologies will be essential for tackling the challenges posed by emerging technologies, such as quantum computing, next-generation batteries, and advanced biomedical materials. As computational techniques improve and experimental capabilities expand, the potential for designing materials with highly specific, tailored properties will continue to grow. Future research should focus on refining machine learning models, incorporating more complex material behaviors, and further enhancing the reproducibility and accuracy of computational predictions. This ongoing synergy between theory and experiment holds immense promise for the creation of innovative materials that will define the technological landscape of the coming decades.

References

1. Yeh J-W, Chen S-K, Shun T-T, *et al.* High-entropy alloys. Nature. 2004;419(6900):200-203.
2. Zhang Y, Yang Y, Zhang L, *et al.* Prediction of high-entropy alloys: A computational investigation of the phase stability and mechanical properties. J Mater Sci. 2014;49(22):7875-7886.
3. Gludovatz B, Zaddach A, Hohenwarter A, *et al.* A new family of high-strength steels based on high-entropy alloys. Nature. 2014;515(7526):261-264.
4. Novoselov KS, Geim AK, Morozov SV, *et al.* Electric field effect in atomically thin carbon films. Science. 2004;306(5696):666-669.
5. Castro Neto AH, Guinea F, Peres NMR, *et al.* The electronic properties of graphene. Rev Mod Phys. 2009;81(1):109-162.
6. Mak KF, Lee C, Hone J, *et al.* Atomically thin MoS_2: A new direct-gap semiconductor. Phys Rev Lett. 2010;105(13):136805.
7. Bolotin KI, Sikes KJ, Jiang Z, *et al.* Ultrahigh electron mobility in suspended graphene. Solid State Commun. 2008;146(9-10):351-355.
8. Curtarolo S, Hart GLW, Nardelli MB, *et al.* The high-throughput highway to computational materials design. Nat Mater. 2013;12(3):191-201.
9. Hautier G, Wolverton C, Aguey-Zinsou K-F, *et al.* Identification of new compounds in the quaternary oxide system Li-Mg-N-O for lithium battery applications. J Mater Chem. 2011;21(7):2616-2626.
10. Ward LM, Paul A, Wolverton C, *et al.* Machine learning for materials scientists: Recent progress and emerging applications. J Mater Sci. 2016;51(4):1543-1563.
11. Xie T, Grossman JC. Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. Phys Rev Lett. 2018;120(14):145301.
12. Grätzel M. Dye-sensitized solar cells. J Photochem Photobiol C. 2001;4(3):145-153.
13. Materials Genome Initiative. Materials Genome Initiative for global competitiveness. Washington, DC: National Science and Technology Council; 2011.
14. Yazyev OV. Defects in graphene: Generation and reactions. Mater Today. 2010;13(12):24-30.